

## N,N'-Dibenzyl-N,N'-dimethyl-N''-(methylsulfonyl)phosphoric triamide

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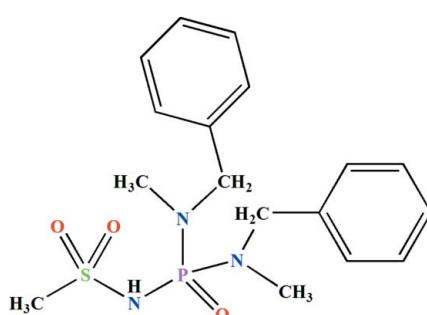
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Key indicators: single-crystal X-ray study;  $T = 296\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$ ;  $R$  factor = 0.032;  $wR$  factor = 0.094; data-to-parameter ratio = 18.4.

In the title compound,  $\text{C}_{17}\text{H}_{24}\text{N}_3\text{O}_3\text{PS}$ , the P and the S atoms are each in a distorted tetrahedral environment and the N atoms display  $sp^2$  character. The phosphoryl group and the NH unit are *anti* with respect to one another. The dihedral angle between the mean planes of the benzene rings is  $31.08(8)^\circ$ . The crystal packing is stabilized by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming an extended chain parallel to the *b* axis.

### Related literature

For phosphoramides having a  $\text{P}(\text{O})(\text{N}(\text{CH}_3)(\text{CH}_2\text{C}_6\text{H}_5))_2$  moiety, see: Pourayoubi *et al.* (2010); Gholivand *et al.* (2005). For bond lengths in a sulfonamide compound, see: Ibrahim *et al.* (2011) and references cited therein.



### Experimental

#### Crystal data

$\text{C}_{17}\text{H}_{24}\text{N}_3\text{O}_3\text{PS}$

$M_r = 381.42$

Orthorhombic,  $P2_12_12_1$   
 $a = 8.5343(4)\text{ \AA}$   
 $b = 10.1800(5)\text{ \AA}$   
 $c = 22.0455(10)\text{ \AA}$   
 $V = 1915.29(16)\text{ \AA}^3$

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.27\text{ mm}^{-1}$   
 $T = 296\text{ K}$   
 $0.47 \times 0.38 \times 0.30\text{ mm}$

#### Data collection

Bruker APEXII CCD  
diffractometer  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 2004)  
 $T_{\min} = 0.700$ ,  $T_{\max} = 0.746$

65627 measured reflections  
4155 independent reflections  
3937 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.060$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.094$   
 $S = 1.08$   
4155 reflections  
226 parameters  
H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.30\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.22\text{ e \AA}^{-3}$   
Absolute structure: Flack (1983),  
1769 Friedel pairs  
Flack parameter: 0.02 (7)

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H}\cdots\text{O1}^i$	0.86	1.91	2.7152 (19)	155
Symmetry code: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$				

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXTL (Sheldrick, 2008) and enCIFer (Allen *et al.*, 2004).

Support of this investigation by Ferdowsi University of Mashhad is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2084).

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## **supplementary materials**

*Acta Cryst.* (2011). E67, o1285 [doi:10.1107/S1600536811015832]

### **N,N'-Dibenzyl-N,N'-dimethyl-N''-(methylsulfonyl)phosphoric triamide**

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#### **Comment**

Structure determination of the title compound,  $\text{CH}_3\text{S}(\text{O})_2\text{NHP(O)}[\text{N}(\text{CH}_3)(\text{CH}_2\text{C}_6\text{H}_5)]_2$  (Fig. 1), was performed as a part of a project in our laboratory on the synthesis of new phosphoramidate compounds having a  $\text{P(O)}[\text{N}(\text{CH}_3)(\text{CH}_2\text{C}_6\text{H}_5)]_2$  moiety (Pourayoubi *et al.*, 2010).

The  $\text{P}=\text{O}$  and  $\text{P}-\text{N}$  bond lengths are comparable to those in similar phosphoramidates of the formula  $\text{XP(O)}[\text{N}(\text{CH}_3)(\text{CH}_2\text{C}_6\text{H}_5)]_2$  [where  $X = \text{Cl}, \text{C}_6\text{H}_5\text{C(O)NH}, \text{CCl}_3\text{C(O)NH}$ ] (Gholivand *et al.*, 2005). The  $\text{P}-\text{N}1$  and  $\text{P}-\text{N}2$  bonds (with bond lengths of 1.6326 (17) Å and 1.6285 (18) Å) are shorter than the  $\text{P}-\text{N}3$  bond (1.6714 (15) Å). The  $\text{S}=\text{O}$  bond lengths of 1.4317 (16) Å & 1.4287 (18) Å are standard for sulfonamide compounds (Ibrahim *et al.*, 2011).

Each of the phosphorus and sulfur atoms has a distorted tetrahedral configuration. The surrounding bond angles are in the range of 104.84 (9)° to 117.02 (9)° around the P atom and 104.79 (12)° to 118.53 (12)° for the S atom. The average of surrounding angles around the tertiary nitrogen atom N2 (which is about 120°) shows that it is bonded in an essentially planar geometry; whereas, the environment of N1 is slightly deviated from planarity (average of bond angles is 118.3°). Furthermore, the S—N3—P angle is 125.05 (9)°. The dihedral angle between the mean planes of the benzene rings is 31.08 (8)°.

The phosphoryl group and the NH unit adopt the *anti* orientations with respect to each other. Crystal packing is stabilized by N—H···O hydrogen bonds, forming an extended chain parallel to the *b* axis (Fig. 2).

#### **Experimental**

$\text{CH}_3\text{S}(\text{O})_2\text{NHP(O)}\text{Cl}_2$  was synthesized from the reaction between phosphorus pentachloride (16.7 mmol) and methanesulfonamide (16.7 mmol) in dry  $\text{CCl}_4$  at 353 K (3 h) and then treated with formic acid 85% (16.7 mmol) at ice bath temperature.

To a solution of  $\text{CH}_3\text{S}(\text{O})_2\text{NHP(O)}\text{Cl}_2$  (2.35 mmol) in dry chloroform (30 ml), a solution of *N*-methylbenzylamine (9.40 mmol) in the same solvent (10 ml) was added at ice bath temperature. After 4 h stirring, the solvent was removed and the product was washed with distilled water and recrystallized from  $\text{CH}_3\text{CN}/\text{CHCl}_3$  at room temperature.

#### **Refinement**

H atoms were placed in calculated positions and included in the refinement in a riding-model approximation with  $\text{CH} = 0.93$ ,  $\text{CH}_2 = 0.97$ ,  $\text{CH}_3 = 0.96$  Å or  $\text{N}—\text{H} = 0.86$  Å with  $U_{\text{iso}}(\text{H})$  parameters equal to  $1.5U_{\text{eq}}(\text{C})$  for methyl H atoms and  $1.2U_{\text{eq}}(\text{C},\text{N})$  for other H atoms.

# supplementary materials

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## Figures

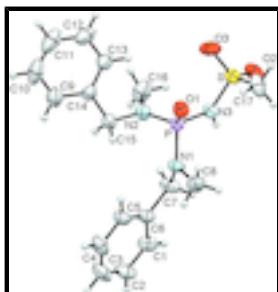


Fig. 1. An ORTEP-style plot of title compound with labeling. Ellipsoids are given at the 50% probability level.

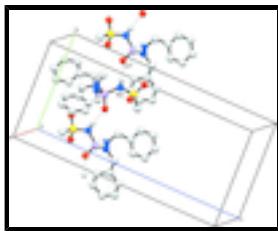


Fig. 2. Partial packing view showing the formation of the chain through N—H···O hydrogen bonds which are shown as dotted lines. H atoms not involved in hydrogen bondings have been omitted for the sake of clarity. [Symmetry code: (i)  $-x, y + 1/2, -z + 1/2$ ]

## *N,N'-Dibenzyl-N,N'-dimethyl- N''-(methylsulfonyl)phosphoric triamide*

### Crystal data

C<sub>17</sub>H<sub>24</sub>N<sub>3</sub>O<sub>3</sub>PS

F(000) = 808

M<sub>r</sub> = 381.42

D<sub>x</sub> = 1.323 Mg m<sup>-3</sup>

Orthorhombic, P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

Mo K $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Hall symbol: P 2ac 2ab

Cell parameters from 9705 reflections

a = 8.5343 (4) Å

$\theta$  = 2.6–29.5°

b = 10.1800 (5) Å

$\mu$  = 0.27 mm<sup>-1</sup>

c = 22.0455 (10) Å

T = 296 K

V = 1915.29 (16) Å<sup>3</sup>

Irregular, colourless

Z = 4

0.47 × 0.38 × 0.30 mm

### Data collection

Bruker APEXII CCD  
diffractometer

4155 independent reflections

Radiation source: fine-focus sealed tube  
graphite

3937 reflections with  $I > 2\sigma(I)$

$\varphi$  and  $\omega$  scans

$R_{\text{int}} = 0.060$

Absorption correction: multi-scan  
(SADABS; Sheldrick, 2004)

$\theta_{\max} = 27.0^\circ, \theta_{\min} = 2.2^\circ$

$T_{\min} = 0.700, T_{\max} = 0.746$

$h = -10 \rightarrow 10$

65627 measured reflections

$k = -13 \rightarrow 13$

$l = -28 \rightarrow 28$

### Refinement

Refinement on  $F^2$

Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.4498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\max} = 0.001$
4155 reflections	$\Delta\rho_{\max} = 0.30 \text{ e \AA}^{-3}$
226 parameters	$\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$
0 restraints	Absolute structure: Flack (1983), <b>1769 Friedel pairs</b>
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (7)

### Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S	-0.14987 (6)	0.66473 (5)	0.33606 (2)	0.03622 (13)
P	0.01450 (6)	0.58351 (4)	0.22593 (2)	0.02755 (11)
O2	-0.1835 (2)	0.78944 (16)	0.36311 (8)	0.0531 (5)
O3	-0.2779 (2)	0.58363 (18)	0.31763 (9)	0.0548 (4)
O1	0.0074 (2)	0.45080 (12)	0.25313 (7)	0.0376 (3)
N2	-0.1005 (2)	0.61222 (17)	0.16850 (8)	0.0374 (4)
N1	0.19197 (19)	0.61606 (16)	0.20271 (8)	0.0357 (4)
C16	-0.2309 (3)	0.7047 (3)	0.16690 (14)	0.0598 (7)
H16A	-0.2367	0.7506	0.2049	0.090*
H16B	-0.3268	0.6577	0.1601	0.090*
H16C	-0.2149	0.7666	0.1346	0.090*
C11	-0.4106 (4)	0.2282 (3)	0.07992 (17)	0.0756 (10)
H11	-0.4817	0.1609	0.0724	0.091*
C10	-0.3104 (4)	0.2678 (3)	0.03513 (15)	0.0733 (9)
H10	-0.3123	0.2269	-0.0026	0.088*
C9	-0.2056 (3)	0.3697 (3)	0.04626 (12)	0.0551 (6)
H9	-0.1402	0.3989	0.0154	0.066*
C14	-0.1979 (2)	0.4282 (2)	0.10302 (9)	0.0377 (4)
C15	-0.0776 (3)	0.5341 (2)	0.11360 (10)	0.0420 (5)
H15A	0.0251	0.4935	0.1155	0.050*
H15B	-0.0780	0.5928	0.0789	0.050*

## supplementary materials

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C7	0.2255 (3)	0.7384 (2)	0.17023 (13)	0.0479 (6)
H7A	0.2714	0.8007	0.1984	0.058*
H7B	0.1277	0.7753	0.1558	0.058*
C6	0.3355 (2)	0.7211 (2)	0.11683 (10)	0.0370 (4)
C1	0.4198 (3)	0.8292 (2)	0.09625 (11)	0.0451 (5)
H1	0.4106	0.9094	0.1161	0.054*
C2	0.5174 (3)	0.8180 (3)	0.04622 (12)	0.0553 (6)
H2	0.5729	0.8907	0.0324	0.066*
C3	0.5322 (3)	0.6990 (3)	0.01694 (11)	0.0621 (7)
H3	0.5980	0.6912	-0.0165	0.074*
N3	-0.0373 (2)	0.69410 (14)	0.27825 (7)	0.0313 (3)
H	-0.0016	0.7726	0.2742	0.038*
C17	-0.0341 (4)	0.5731 (3)	0.38565 (11)	0.0583 (7)
H17A	0.0536	0.6251	0.3986	0.087*
H17B	0.0031	0.4958	0.3653	0.087*
H17C	-0.0952	0.5480	0.4203	0.087*
C8	0.3248 (3)	0.5572 (3)	0.23501 (12)	0.0588 (7)
H8A	0.2915	0.4778	0.2546	0.088*
H8B	0.3631	0.6179	0.2649	0.088*
H8C	0.4069	0.5375	0.2067	0.088*
C5	0.3510 (3)	0.6022 (2)	0.08697 (10)	0.0448 (5)
H5	0.2952	0.5292	0.1002	0.054*
C4	0.4499 (3)	0.5922 (3)	0.03725 (11)	0.0578 (6)
H4	0.4604	0.5120	0.0175	0.069*
C13	-0.2991 (3)	0.3855 (2)	0.14752 (11)	0.0478 (5)
H13	-0.2951	0.4233	0.1859	0.057*
C12	-0.4069 (3)	0.2868 (3)	0.13576 (15)	0.0633 (8)
H12	-0.4766	0.2604	0.1658	0.076*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S	0.0438 (3)	0.0249 (2)	0.0400 (2)	-0.0002 (2)	0.0118 (2)	0.00027 (19)
P	0.0334 (2)	0.01673 (19)	0.0325 (2)	-0.00014 (17)	0.00382 (18)	-0.00090 (16)
O2	0.0683 (12)	0.0342 (8)	0.0568 (9)	0.0053 (8)	0.0255 (9)	-0.0081 (7)
O3	0.0429 (8)	0.0435 (9)	0.0780 (12)	-0.0137 (8)	0.0150 (8)	-0.0002 (8)
O1	0.0544 (8)	0.0169 (6)	0.0414 (7)	-0.0007 (6)	0.0042 (7)	-0.0001 (5)
N2	0.0398 (9)	0.0332 (9)	0.0393 (8)	0.0046 (7)	-0.0017 (7)	-0.0013 (7)
N1	0.0336 (8)	0.0301 (8)	0.0433 (9)	0.0012 (7)	0.0082 (7)	-0.0015 (7)
C16	0.0598 (15)	0.0479 (13)	0.0715 (17)	0.0193 (12)	-0.0217 (14)	-0.0054 (13)
C11	0.083 (2)	0.0558 (17)	0.088 (2)	-0.0198 (16)	-0.0378 (19)	0.0022 (16)
C10	0.092 (2)	0.0602 (17)	0.0673 (18)	0.0035 (17)	-0.0323 (18)	-0.0242 (15)
C9	0.0606 (15)	0.0588 (15)	0.0460 (12)	0.0044 (12)	-0.0048 (11)	-0.0095 (11)
C14	0.0360 (10)	0.0378 (10)	0.0394 (10)	0.0035 (9)	-0.0055 (8)	-0.0014 (8)
C15	0.0426 (11)	0.0498 (12)	0.0335 (10)	-0.0064 (10)	0.0038 (9)	-0.0025 (9)
C7	0.0481 (12)	0.0276 (10)	0.0681 (15)	-0.0014 (9)	0.0255 (12)	-0.0040 (10)
C6	0.0321 (10)	0.0344 (10)	0.0445 (11)	0.0045 (8)	0.0053 (9)	0.0037 (8)
C1	0.0411 (11)	0.0380 (11)	0.0562 (13)	0.0045 (10)	0.0081 (10)	0.0102 (10)

C2	0.0521 (13)	0.0568 (14)	0.0572 (14)	0.0027 (12)	0.0138 (12)	0.0231 (12)
C3	0.0648 (17)	0.0809 (19)	0.0404 (12)	0.0116 (15)	0.0189 (12)	0.0099 (13)
N3	0.0405 (8)	0.0157 (6)	0.0376 (8)	-0.0018 (6)	0.0083 (7)	-0.0012 (6)
C17	0.090 (2)	0.0473 (13)	0.0379 (11)	0.0056 (14)	-0.0010 (12)	0.0081 (10)
C8	0.0402 (12)	0.0805 (19)	0.0558 (14)	0.0078 (13)	-0.0026 (11)	-0.0025 (13)
C5	0.0418 (11)	0.0420 (12)	0.0505 (12)	0.0027 (10)	0.0077 (10)	-0.0021 (9)
C4	0.0680 (16)	0.0596 (16)	0.0456 (12)	0.0113 (13)	0.0119 (11)	-0.0092 (12)
C13	0.0491 (12)	0.0486 (13)	0.0456 (12)	-0.0100 (10)	-0.0059 (9)	0.0022 (10)
C12	0.0523 (15)	0.0623 (17)	0.0751 (18)	-0.0195 (13)	-0.0145 (13)	0.0149 (14)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

S—O3	1.4287 (18)	C15—H15B	0.9700
S—O2	1.4317 (16)	C7—C6	1.516 (3)
S—N3	1.6236 (16)	C7—H7A	0.9700
S—C17	1.744 (3)	C7—H7B	0.9700
P—O1	1.4794 (13)	C6—C5	1.384 (3)
P—N2	1.6285 (18)	C6—C1	1.390 (3)
P—N1	1.6326 (17)	C1—C2	1.387 (3)
P—N3	1.6714 (15)	C1—H1	0.9300
N2—C16	1.458 (3)	C2—C3	1.378 (4)
N2—C15	1.461 (3)	C2—H2	0.9300
N1—C7	1.465 (3)	C3—C4	1.369 (4)
N1—C8	1.467 (3)	C3—H3	0.9300
C16—H16A	0.9600	N3—H	0.8600
C16—H16B	0.9600	C17—H17A	0.9600
C16—H16C	0.9600	C17—H17B	0.9600
C11—C12	1.368 (5)	C17—H17C	0.9600
C11—C10	1.367 (5)	C8—H8A	0.9600
C11—H11	0.9300	C8—H8B	0.9600
C10—C9	1.392 (4)	C8—H8C	0.9600
C10—H10	0.9300	C5—C4	1.387 (3)
C9—C14	1.387 (3)	C5—H5	0.9300
C9—H9	0.9300	C4—H4	0.9300
C14—C13	1.378 (3)	C13—C12	1.387 (4)
C14—C15	1.507 (3)	C13—H13	0.9300
C15—H15A	0.9700	C12—H12	0.9300
O3—S—O2	118.53 (12)	C6—C7—H7A	108.8
O3—S—N3	109.61 (10)	N1—C7—H7B	108.8
O2—S—N3	106.39 (9)	C6—C7—H7B	108.8
O3—S—C17	107.61 (13)	H7A—C7—H7B	107.7
O2—S—C17	109.08 (12)	C5—C6—C1	119.2 (2)
N3—S—C17	104.79 (12)	C5—C6—C7	121.98 (19)
O1—P—N2	117.02 (9)	C1—C6—C7	118.82 (19)
O1—P—N1	110.51 (9)	C2—C1—C6	120.3 (2)
N2—P—N1	106.20 (9)	C2—C1—H1	119.8
O1—P—N3	108.94 (8)	C6—C1—H1	119.8
N2—P—N3	104.84 (9)	C3—C2—C1	120.0 (2)
N1—P—N3	108.98 (8)	C3—C2—H2	120.0

## supplementary materials

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C16—N2—C15	115.69 (19)	C1—C2—H2	120.0
C16—N2—P	126.49 (17)	C4—C3—C2	119.8 (2)
C15—N2—P	117.76 (15)	C4—C3—H3	120.1
C7—N1—C8	115.7 (2)	C2—C3—H3	120.1
C7—N1—P	120.48 (14)	S—N3—P	125.05 (9)
C8—N1—P	118.83 (16)	S—N3—H	117.5
N2—C16—H16A	109.5	P—N3—H	117.5
N2—C16—H16B	109.5	S—C17—H17A	109.5
H16A—C16—H16B	109.5	S—C17—H17B	109.5
N2—C16—H16C	109.5	H17A—C17—H17B	109.5
H16A—C16—H16C	109.5	S—C17—H17C	109.5
H16B—C16—H16C	109.5	H17A—C17—H17C	109.5
C12—C11—C10	120.5 (3)	H17B—C17—H17C	109.5
C12—C11—H11	119.8	N1—C8—H8A	109.5
C10—C11—H11	119.8	N1—C8—H8B	109.5
C11—C10—C9	119.6 (3)	H8A—C8—H8B	109.5
C11—C10—H10	120.2	N1—C8—H8C	109.5
C9—C10—H10	120.2	H8A—C8—H8C	109.5
C14—C9—C10	120.6 (3)	H8B—C8—H8C	109.5
C14—C9—H9	119.7	C6—C5—C4	119.9 (2)
C10—C9—H9	119.7	C6—C5—H5	120.1
C13—C14—C9	118.5 (2)	C4—C5—H5	120.1
C13—C14—C15	122.87 (19)	C3—C4—C5	120.8 (2)
C9—C14—C15	118.6 (2)	C3—C4—H4	119.6
N2—C15—C14	115.23 (18)	C5—C4—H4	119.6
N2—C15—H15A	108.5	C14—C13—C12	120.8 (2)
C14—C15—H15A	108.5	C14—C13—H13	119.6
N2—C15—H15B	108.5	C12—C13—H13	119.6
C14—C15—H15B	108.5	C11—C12—C13	119.9 (3)
H15A—C15—H15B	107.5	C11—C12—H12	120.0
N1—C7—C6	113.73 (16)	C13—C12—H12	120.0
N1—C7—H7A	108.8		
O1—P—N2—C16	114.6 (2)	P—N1—C7—C6	-138.44 (18)
N1—P—N2—C16	-121.5 (2)	N1—C7—C6—C5	24.7 (3)
N3—P—N2—C16	-6.2 (2)	N1—C7—C6—C1	-157.2 (2)
O1—P—N2—C15	-62.24 (18)	C5—C6—C1—C2	0.3 (3)
N1—P—N2—C15	61.66 (17)	C7—C6—C1—C2	-177.8 (2)
N3—P—N2—C15	176.96 (15)	C6—C1—C2—C3	-0.5 (4)
O1—P—N1—C7	175.63 (16)	C1—C2—C3—C4	0.3 (4)
N2—P—N1—C7	47.76 (19)	O3—S—N3—P	-41.70 (16)
N3—P—N1—C7	-64.70 (18)	O2—S—N3—P	-170.99 (13)
O1—P—N1—C8	-30.5 (2)	C17—S—N3—P	73.54 (16)
N2—P—N1—C8	-158.39 (18)	O1—P—N3—S	-25.84 (16)
N3—P—N1—C8	89.15 (19)	N2—P—N3—S	100.16 (13)
C12—C11—C10—C9	-0.9 (5)	N1—P—N3—S	-146.48 (13)
C11—C10—C9—C14	2.4 (5)	C1—C6—C5—C4	0.1 (4)
C10—C9—C14—C13	-1.7 (4)	C7—C6—C5—C4	178.2 (2)
C10—C9—C14—C15	177.4 (2)	C2—C3—C4—C5	0.2 (4)
C16—N2—C15—C14	-72.4 (3)	C6—C5—C4—C3	-0.4 (4)

## supplementary materials

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P—N2—C15—C14	104.8 (2)	C9—C14—C13—C12	-0.3 (4)
C13—C14—C15—N2	-15.1 (3)	C15—C14—C13—C12	-179.4 (2)
C9—C14—C15—N2	165.9 (2)	C10—C11—C12—C13	-1.2 (5)
C8—N1—C7—C6	66.9 (3)	C14—C13—C12—C11	1.8 (4)

*Hydrogen-bond geometry (Å, °)*

D—H···A	D—H	H···A	D···A	D—H···A
N3—H···O1 <sup>i</sup>	0.86	1.91	2.7152 (19)	155

Symmetry codes: (i)  $-x, y+1/2, -z+1/2$ .

## supplementary materials

Fig. 1

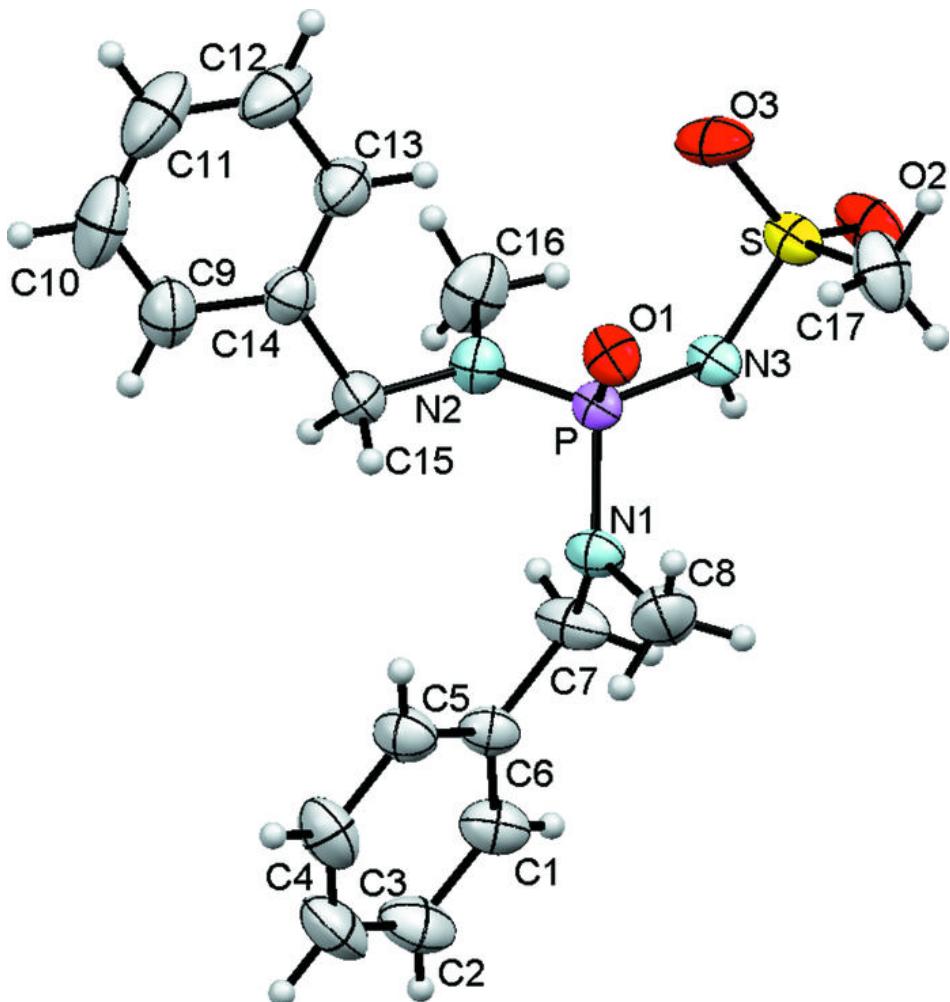


Fig. 2

